

10/015, 128

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1204bxd

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 JAN 27 Source of Registration (SR) information in REGISTRY updated  
and searchable  
NEWS 4 JAN 27 A new search aid, the Company Name Thesaurus, available in  
CA/Caplus  
NEWS 5 FEB 05 German (DE) application and patent publication number format  
changes  
NEWS 6 MAR 03 MEDLINE and LMedLINE reloaded  
NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded  
NEWS 8 MAR 03 FRANCEPAT now available on STN  
NEWS 9 MAR 29 Pharmaceutical Substances (PS) now available on STN  
NEWS 10 MAR 29 WPIFV now available on STN  
NEWS 11 MAR 29 No connect hour charges in WPIFV until May 1, 2004  
NEWS 12 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA  
NEWS 13 APR 26 PROMT: New display field available  
NEWS 14 APR 26 FIPAT/IFIUDB/IFICDB: New super search and display field  
available  
NEWS 15 APR 26 LITAlert now available on STN  
NEWS 16 APR 27 NLDB: New search and display fields available  
  
NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 13 APRIL 2004  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that  
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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 17:12:07 ON 27 APR 2004

=> FIL STNGUIDE  
COST IN U.S. DOLLARS

SINCE FILE TOTAL  
ENTRY SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'STNGUIDE' ENTERED AT 17:12:11 ON 27 APR 2004  
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Apr 23, 2004 (20040423/UP).

=> FIL HOME  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.06	0.27

FULL ESTIMATED COST

FILE 'HOME' ENTERED AT 17:12:14 ON 27 APR 2004

=> fil reg  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.48

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 17:12:24 ON 27 APR 2004  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 26 APR 2004 HIGHEST RN 676992-14-6  
DICTIONARY FILE UPDATES: 26 APR 2004 HIGHEST RN 676992-14-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

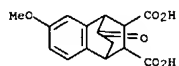
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> s 29073-46-9/rn  
L1 1 29073-46-9/RN

=> d l1

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 29073-46-9 REGISTRY  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1 $\alpha$ ,2 $\beta$ ,3 $\alpha$ ,4 $\alpha$   
MF 1 $\alpha$ ,2 $\beta$ ,3 $\alpha$ ,4 $\alpha$ -tetrahydro-6-methoxy-8-oxo-, (±)- [8CI] (CA INDEX NAME)  
C15 H14 O6  
LC STN Files: CA, CAPLUS

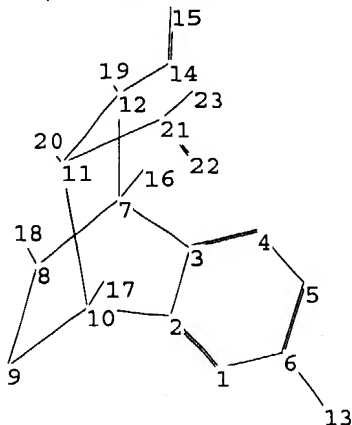
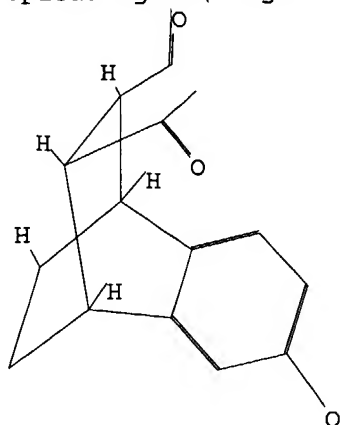


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>

Uploading C:\Program Files\Stnexp\Queries\10015828.str



chain nodes :

13 14 15 16 17 18 19 20 21 22 23

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

6-13 7-16 8-18 10-17 11-20 11-21 12-14 12-19 14-15 21-22 21-23

ring bonds :

1-2 1-6 2-3 2-10 3-4 3-7 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

2-10 3-7 6-13 7-8 7-12 8-9 9-10 10-11 11-12 14-15 21-22

exact bonds :

7-16 8-18 10-17 11-20 11-21 12-14 12-19 21-23

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

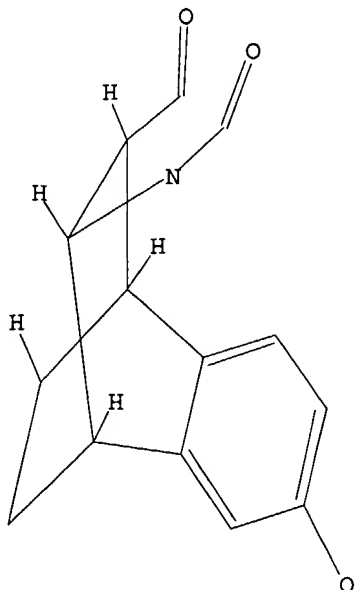
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS

L2 STRUCTURE UPLOADED

=> d query

L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l2

SAMPLE SEARCH INITIATED 17:27:35 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 165 TO ITERATE

100.0% PROCESSED 165 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2530 TO 4070  
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L2

=> s l2 full

FULL SEARCH INITIATED 17:27:39 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 3373 TO ITERATE

100.0% PROCESSED 3373 ITERATIONS  
SEARCH TIME: 00.00.01

19 ANSWERS

L4 19 SEA SSS FUL L2

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

167.69

168.17

FILE 'CAPLUS' ENTERED AT 17:27:42 ON 27 APR 2004  
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FILE COVERS 1907 - 27 Apr 2004 VOL 140 ISS 18  
FILE LAST UPDATED: 26 Apr 2004 (20040426/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l4

L5                    2 L4

=> d l5 1-2 abs ibib hitstr

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [R1 = NR8COR9, NR8CO2R9, NR8CON(R9)2, COR9, CO2R9, CON(R9)2; R2 = OR9, N(R9)2; R3 = H, halo, OH, protected-OH, NH2, protected-NH2, alkyl, haloalkyl; R4-5 = R9, OR9, N(R9)2, N=NR9, R4, R5 may together form =O, =C(R8)2, NR10 or R4-5 together with the carbon to which they are both attached form spiro carbocyclic or heterocyclic ring; R6 = H, inorg. groups having 1-8 atoms selected from boron, sulfur, phosphorus, silicon, hydrogen, and organic groups having 1-20 carbons, optionally containing 1-4 heteroatoms selected from nitrogen, oxygen and silicon; R7 = halo, OH, protected-OH, NH2, protected-NH2, alkyl, haloalkyl; R8 = H, alkyl, aryl, heteroalkyl; R9 = H, organic groups having 1-30 carbons with the provision that two R9 groups both joined to common atom may be joined together so as to form ring with the common atom; R10 = R9, OR9, N(R9)2, NHCOR9, NHCOR9R9, NHCNHR9; n is 0-2; with the proviso that when R6 = H, R4-5 together form =O and R1 = CO2R2, then R2 is not OCH3] were prepared. For instance, 2,7-dihydroxynaphthalene was reacted with maleic anhydride (1,2-dichlorobenzene/PhMe, 110°C, 3 days) to afford the bicyclobenzocyclobutane adduct (16% yield). This anhydride was reacted with 2-(trimethylsilyl)ethanol affording a 1:1 mixture of regio isomers which was isolated as the dicyclohexylamine (DCA) salt (93% yield). The DCA salt was treated with 2M HCl permitting the isolation of the free regioisomers which were then converted to the isopropylamine salts and crystallized affording the desired regioisomer as a 87/16 mixture. Further crystallization and liberation of the acid ester afforded II as a white solid in 30% overall yield with 98.2% purity by HPLC. Also described is a process of preparing a combinatorial library of I from III [linker = e.g., O-CH2-C6H5-O-CH2CONH; SS = solid support; PGI = protecting group, e.g., O-allyl; PG2 = protecting group, e.g., OCH2CH2TMS]. The method involves removal of PG1 (PG1 = O-allyl, (Ph)34Pd/N-methylaniline) in the presence of PG2 (PG2 = OCH2CH2TMS, TBAF) and subsequent amidation with a plurality of amines; removal of PG2 and amidation with a plurality of amines and removal of the linker (TFAAq) to liberate the corresponding bis(amides). A library of 1152 bis(amides) were prepared in this manner. Compds. of the invention were evaluated for inhibition of apoptosis and NFkB. I are useful for inhibiting cellular events involving TNF-α and IL-8, and in the treatment of inflammation events in general.

ACCESSION NUMBER: 2002:504796 CAPLUS  
DOCUMENT NUMBER: 137:78768  
TITLE: Preparation and use of benzobicyclobutanes as inhibitors of TNF-α, IL-8 and for treating inflammation  
INVENTOR(S): Jackson, Randy W.; Darwish, Ihab; Howbert, J. Jeffery

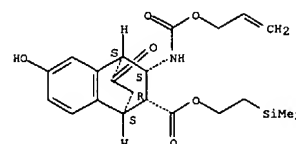
L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
PATENT ASSIGNEE(S): Celltech R & D, Inc., USA  
SOURCE: PCT Int. Appl., 200 pp.  
CODEN: FIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002051851	A2	20020704	WO 2001-US47993	20011211
WO 2002051851	A3	20030123		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, ZM, ZY, AA, AB, AC, AD, AE, AF, AG, AH, AI, AJ, AK, AL, AM, AN, AO, AP, AQ, AR, AS, AT, AU, AV, AW, AX, AY, AZ, BA, BB, BC, BD, BE, BF, BG, BH, BI, BJ, BK, BL, BM, BN, BO, BP, BQ, BR, BS, BT, BU, BV, BW, BY, BZ, CA, CB, CC, CD, CE, CF, CG, CH, CI, CJ, CK, CL, CM, CN, CO, CP, CQ, CR, CS, CT, CU, CV, CW, CX, CY, CZ, DA, DB, DD, DE, DF, DG, DH, DI, DJ, DK, DL, DM, DN, DO, DP, DQ, DR, DS, DT, DU, DV, DW, DX, DY, DZ, EA, EB, EC, ED, EE, EF, EG, EH, EI, EJ, EK, EL, EM, EN, EO, EP, EQ, ER, ES, ET, EU, EV, EW, EX, EY, EZ, FA, FB, FC, FD, FE, FF, FG, FH, FI, FJ, FK, FL, FM, FN, FO, FP, FQ, FR, FS, FT, FU, FV, FW, FX, FY, FZ, GA, GB, GC, GD, GE, GF, GH, GI, GJ, GK, GL, GM, GN, GP, GQ, GR, GS, GT, GU, GV, GW, GX, GY, GZ, HA, HB, HC, HD, HE, HF, HG, HH, HI, HJ, HK, HL, HM, HN, HO, HP, HQ, HR, HS, HT, HU, HV, HW, HX, HY, HZ, IA, IB, IC, ID, IE, IF, IG, IH, II, IJ, IK, IL, IM, IN, IO, IP, IQ, IR, IS, IT, IU, IV, IW, IX, IY, IZ, JA, JB, JC, JD, JE, JF, JG, JH, JI, JJ, JK, JL, JM, JN, JO, JP, JQ, JR, JS, JT, JU, JV, JW, JX, JY, JZ, KA, KB, KC, KD, KE, KF, KG, KH, KI, KJ, KK, KL, KM, KN, KO, KP, KQ, KR, KS, KT, KU, KV, KW, KX, KY, KZ, LA, LB, LC, LD, LE, LF, LG, LH, LI, LJ, LK, LM, LN, LO, LP, LQ, LR, LS, LT, LU, LV, LW, LX, LY, LZ, MA, MB, MC, MD, ME, MF, MG, MH, MI, MJ, MK, ML, MN, MO, MP, MQ, MR, MS, MT, MU, MV, MW, MX, MY, MZ, NA, NB, NC, ND, NE, NF, NG, NH, NI, NJ, NK, NL, NM, NO, NP, NQ, NR, NS, NT, NU, NV, NW, NX, NY, NZ, OA, OB, OC, OD, OE, OF, OG, OH, OI, OJ, OK, OL, OM, ON, OO, OP, OQ, OR, OS, OT, OU, OV, OW, OX, OY, OZ, PA, PB, PC, PD, PE, PF, PG, PH, PI, PJ, PK, PL, PM, PN, PO, PP, PQ, PR, PS, PT, PU, PV, PW, PX, PY, PZ, QA, QB, QC, QD, QE, QF, QG, QH, QI, QJ, QK, QL, QM, QN, QO, QP, QQ, QR, QS, QT, QU, QV, QW, QX, QY, QZ, RA, RB, RC, RD, RE, RF, RG, RH, RI, RJ, RK, RL, RM, RN, RO, RP, RQ, RR, RS, RT, RU, RV, RW, RX, RY, RZ, SA, SB, SC, SD, SE, SF, SG, SH, SI, SJ, SK, SL, SM, SN, SO, SP, SQ, SR, SS, ST, SU, SV, SW, SX, SY, SZ, TA, TB, TC, TD, TE, TF, TG, TH, TI, TJ, TK, TL, TM, TN, TO, TP, TQ, TR, TS, TT, TU, TV, TW, TX, TY, TZ, UA, UB, UC, UD, UE, UF, UG, UH, UI, UJ, UK, UL, UM, UN, UO, UP, UQ, UR, US, UT, UU, UV, UW, UX, UY, UZ, VA, VB, VC, VD, VE, VF, VG, VH, VI, VJ, VK, VL, VM, VN, VO, VP, VQ, VR, VS, VT, VU, VV, VW, VX, VY, VZ, WA, WB, WC, WD, WE, WF, WG, WH, WI, WJ, WK, WL, WM, WN, WO, WP, WQ, WR, WS, WT, WU, WV, WW, WX, WY, WZ, XA, XB, XC, XD, XE, XF, XG, XH, XI, XJ, XK, XL, XM, XN, XO, XP, XQ, XR, XS, XT, XU, XV, XW, XX, XY, XZ, YA, YB, YC, YD, YE, YF, YG, YH, YI, YJ, YK, YL, YM, YN, YO, YP, YQ, YR, YS, YT, YU, YV, YW, YX, YY, YZ, ZA, ZB, ZC, ZD, ZE, ZF, ZG, ZH, ZI, ZJ, ZK, ZL, ZM, ZN, ZO, ZP, ZQ, ZR, ZS, ZT, ZU, ZV, ZW, ZX, ZY, ZZ.

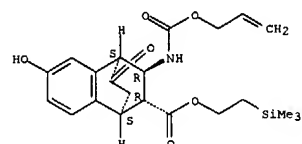
US 2003069305 A1 20030410 US 2001-15828 20011211  
PRIORITY APPLN. INFO.: US 2000-257532P P 20001222  
OTHER SOURCE(S): MARPAT 137:78768  
IT 439798-63-7P 439798-84-2P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(drug; preparation of benzobicyclobutanes derived from Diels-Alder adduct of 2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TNF-α, IL-8)  
RN 439798-63-7 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-3-[(2-propenyloxy)carbonyl]amino]-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



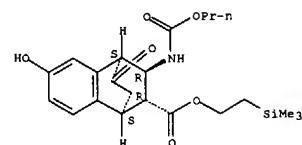
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CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-3-[(2-propenyloxy)carbonyl]amino]-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



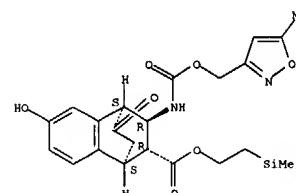
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(drug; preparation of benzobicyclobutanes derived from Diels-Alder adduct of 2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TNF-α, IL-8)  
RN 439798-80-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-3-[(propoxy)carbonyl]amino]-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



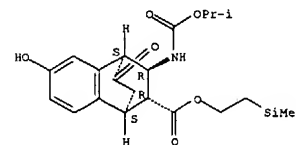
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Relative stereochemistry.



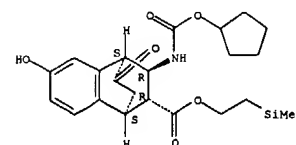
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Relative stereochemistry.



RN 439798-83-1 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 3-[[[(2,3-dihydro-1H-inden-2-yl)oxy]carbonyl]amino]-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

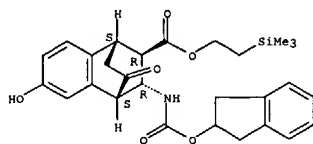
Relative stereochemistry.



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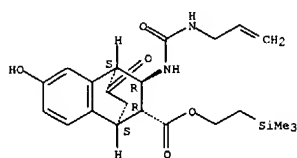
L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS ON STN (Continued)  
2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



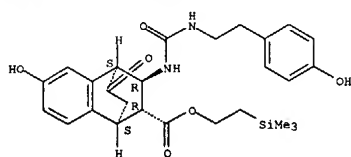
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Relative stereochemistry.



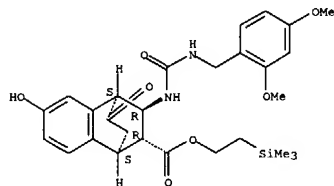
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CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-3-[[[2-(4-hydroxyphenyl)ethyl]amino]carbonyl]amino]-9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



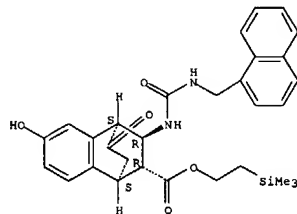
RN 439798-88-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-3-[(4-morpholinylcarbonyl)amino]-9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS ON STN (Continued)



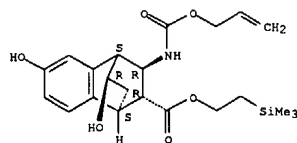
RN 439798-91-1 CAPLUS  
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Relative stereochemistry.



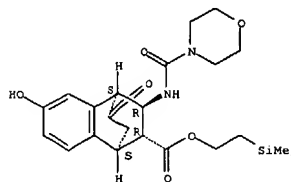
RN 439799-36-7 CAPLUS  
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Relative stereochemistry.



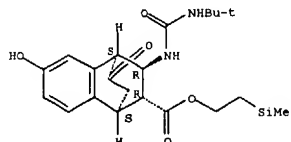
L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS ON STN (Continued)  
(1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 439798-89-7 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 3-[[[1,1-dimethylethyl]amino]carbonyl]amino]-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 439798-90-0 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 3-[[[2,4-dimethoxyphenyl]methyl]amino]carbonyl]amino]-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

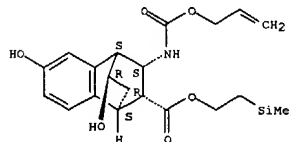
Relative stereochemistry.



L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS ON STN (Continued)

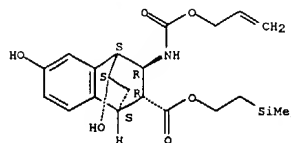
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Relative stereochemistry.



RN 439799-80-1 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-3-[[[2-(propenyloxy)carbonyl]amino]-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

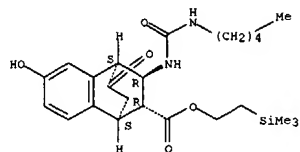


RN 439800-25-6 CAPLUS  
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Relative stereochemistry.



L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



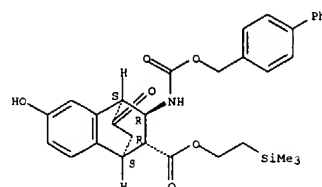
L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

AB A novel series of TNF- $\alpha$  inhibitors based on a benzobicyclooctane scaffold was reported. The compds. displayed good potency in inhibiting TNF- $\alpha$  induced apoptosis and NF $\kappa$ B activation. Addnl., they were selective for TNF- $\alpha$  as they did not inhibit apoptosis induced by soluble Fas ligand. The compds. described here can act as leads for future medicinal chemical efforts and may also be useful tools for elucidating the TNF- $\alpha$  signaling pathway.

ACCESSION NUMBER: 2002:211239 CAPLUS  
DOCUMENT NUMBER: 137:288467  
TITLE: Benzobicyclooctanes as novel inhibitors of TNF- $\alpha$  signaling  
AUTHOR(S): Jackson, Randy W.; Gelinas, Richard; Baughman, Ted A.; Cox, Thomas; Howbert, J. Jeffrey; Kucera, Kristin A.; Latham, John A.; Ramsdell, Fred; Singh, Devinder; Darwish, Ihab S.  
CORPORATE SOURCE: Department of Chemical Genomics, Celltech R&D, Inc., Bothell, WA, 98021, USA  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(7), 1093-1097  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

IT 468086-82-0P 468086-83-1P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(benzobicyclooctanes as novel inhibitors of TNF- $\alpha$  signaling)  
RN 468086-82-0 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 3-[[[1,1'-biphenyl]-4-ylmethoxy]carbonylamino]-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

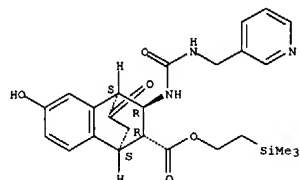
Relative stereochemistry.



RN 468086-83-1 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-3-[[[3-pyridinylmethyl]amino]carbonylamino]-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

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SINCE FILE	TOTAL
ENTRY	SESSION
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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STRUCTURE FILE UPDATES: 26 APR 2004 HIGHEST RN 676992-14-6

DICTIONARY FILE UPDATES: 26 APR 2004 HIGHEST RN 676992-14-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

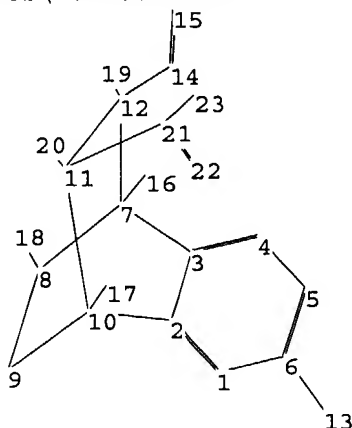
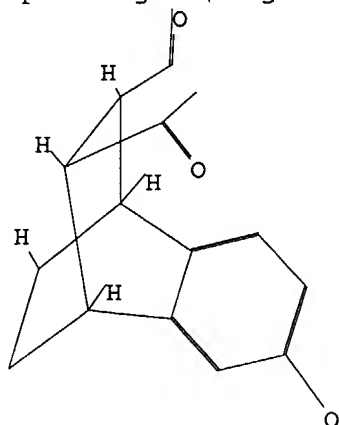
Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10015828.str



chain nodes :

13 14 15 16 17 18 19 20 21 22 23

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

6-13 7-16 8-18 10-17 11-20 11-21 12-14 12-19 14-15 21-22 21-23

ring bonds :

1-2 1-6 2-3 2-10 3-4 3-7 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

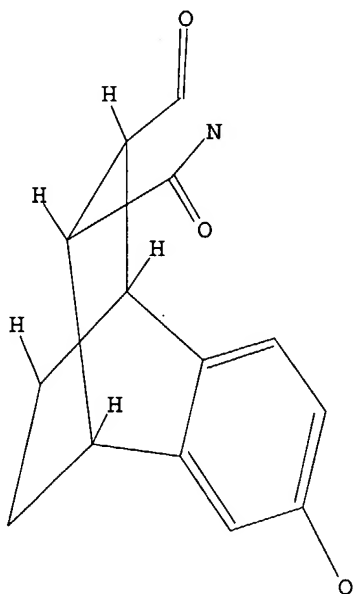
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 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS

L6 STRUCTURE UPLOADED

=> d query

L6 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 17:32:36 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 60 TO ITERATE

100.0% PROCESSED 60 ITERATIONS  
 SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 736 TO 1664  
 PROJECTED ANSWERS: 0 TO 0

L7                    0 SEA SSS SAM L6

=> s l6 full  
FULL SEARCH INITIATED 17:32:41 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1196 TO ITERATE

100.0% PROCESSED        1196 ITERATIONS                    7 ANSWERS  
SEARCH TIME: 00.00.01

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CA SUBSCRIBER PRICE	0.00	-1.39

FILE 'CAPLUS' ENTERED AT 17:32:44 ON 27 APR 2004  
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FILE COVERS 1907 - 27 Apr 2004 VOL 140 ISS 18  
FILE LAST UPDATED: 26 Apr 2004 (20040426/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l8  
L9                    2 L8

=> d l9 1-2 abs ibib hitstr

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [R1 = NR8COR9, NR8CO2R9, NR8CON(R9)2, COR9, CO2R9, CON(R9)2; R2 = OR9, N(R9)2; R3 = H, halo, OH, protected-OH, NH2, protected-NH2, alkyl, haloalkyl; R4-5 = R9, OR9, N(R9)2, N=NR9, R4, R5 may together form =O, =C(R8)2, NR10 or R4-5 together with the carbon to which they are both attached form spiro carbocyclic or heterocyclic ring; R6 = H, inorg. groups having 1-8 atoms selected from boron, sulfur, phosphorus, silicon, hydrogen, and organic groups having 1-20 carbons, optionally containing 1-4 heteroatoms selected from nitrogen, oxygen and silicon; R7 = halo, OH, protected-OH, NH2, protected-NH2, alkyl, haloalkyl; R8 = H, alkyl, aryl, heteroalkyl; R9 = H, organic groups having 1-30 carbons with the provision that two R9 groups both joined to common atom may be joined together so as to form ring with the common atom; R10 = R9, OR9, N(R9)2, NHCOR9, NHCOR9, NHCNHR9; n is 0-2; with the proviso that when R6 = H, R4-5 together form =O and R1 = CO2R2, then R2 is not OCH3] were prepared. For instance, 2,7-dihydroxynaphthalene was reacted with maleic anhydride (1,2-dichlorobenzene/PhMe, 110°C, 3 days) to afford the bicyclobenzocyclobutane adduct (16% yield). This anhydride was reacted with 2-(trimethylsilyl)ethanol affording a 1:1 mixture of regio isomers which was isolated as the dicyclohexylamine (DCA) salt (93% yield). The DCA salt was treated with 2M HCl permitting the isolation of the free regioisomers which were then converted to the isopropylamine salts and crystallized affording the desired regioisomer as a 87/16 mixture. Further crystallization and liberation of the acid ester afforded II as a white solid in 30% overall yield with 98.2% purity by HPLC. Also described is a process of preparing a combinatorial library of I from III [linker = e.g., O-CH2-C6H5-O-CH2CONH; SS = solid support; PG1 = protecting group, e.g., O-allyl; PG2 = protecting group, e.g., OCH2CH2TMS]. The method involves removal of PG1 (PG1 = O-allyl, (Ph3)4Pd/N-methylaniline) in the presence of PG2 (PG2 = OCH2CH2TMS, TBAF) and subsequent amidation with a plurality of amines; removal of PG2 and amidation with a plurality of amines and removal of the linker (TPAaq) to liberate the corresponding bis(amides). A library of 1152 bis(amides) were prepared in this manner. Comps. of the invention were evaluated for inhibition of apoptosis and NFkB. I are useful for inhibiting cellular events involving TNF-α and IL-8, and in the treatment of inflammation events in general.

ACCESSION NUMBER: 2002:504796 CAPLUS  
DOCUMENT NUMBER: 137:78768  
TITLE: Preparation and use of benzobicyclobutanes as inhibitors of TNF-α, IL-8 and for treating inflammation  
INVENTOR(S): Jackson, Randy W.; Darwish, Ihab; Baughman, Ted A.; Howbert, J. Jeffery

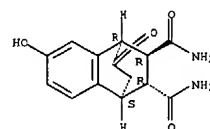
L9 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
PATENT ASSIGNEE(S): Celltech R & D, Inc., USA  
SOURCE: PCT Int. Appl., 200 pp.  
CODEN: FIKXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002051851	A2	20020704	WO 2001-US47993	20011211
WO 2002051851	A3	20030123		

W: AS, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003069305 A1 20030410 US 2001-15828 20011211  
PRIORITY APPL. INFO.: MARPAT 137:78768  
OTHER SOURCE(S):  
IT 439799-73-2DP, combinatorial library of amide derivs.  
RI: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)  
(drug; preparation of benzobicyclobutanes derived from Diels-Alder adduct of 2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TNF-α, IL-8)  
RN 439799-73-2 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxamide, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

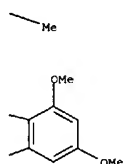
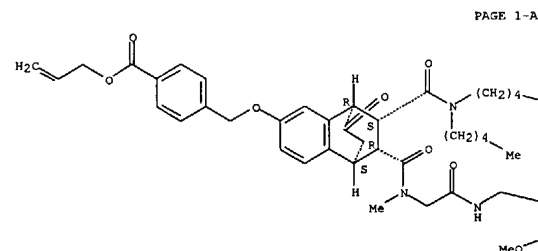
Relative stereochemistry.



IT 439798-66-OP 439798-67-1P 439798-79-5P  
RI: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(drug; preparation of benzobicyclobutanes derived from Diels-Alder adduct of 2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TNF-α, IL-8)  
RN 439798-66-0 CAPLUS  
CN Benzoic acid, 4-[[[(1R,2S,3R,4S)-3-[[[dipentylamino]carbonyl]-1,2,3,4-

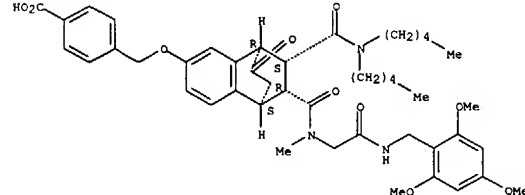
tetrahydro-2-[[[methyl(2-oxo-2-[[[(2,4,6-trimethoxyphenyl)methyl]amino]ethyl]amino]carbonyl]-9-oxo-1,4-ethanonaphthalene-6-yl]oxy]methyl]-, 2-propenyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



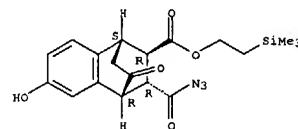
RN 439798-67-1 CAPLUS  
CN Benzoic acid, 4-[[[(1R,2S,3R,4S)-3-[[[dipentylamino]carbonyl]-1,2,3,4-tetrahydro-2-[[[methyl(2-oxo-2-[[[(2,4,6-trimethoxyphenyl)methyl]amino]ethyl]amino]carbonyl]-9-oxo-1,4-ethanonaphthalene-6-yl]oxy]methyl]-, rel- (9CI) (CA INDEX NAME)]

Relative stereochemistry.



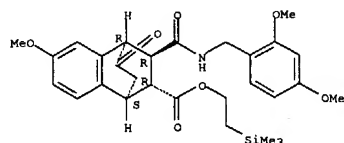
RN 439798-79-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 3-[[[(2,4,6-trimethoxyphenyl)methyl]amino]carbonyl]-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



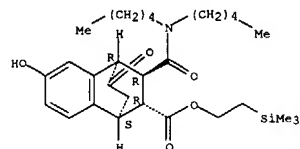
IT 439798-70-6P 439798-71-7P 439919-18-3P  
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(drug; preparation of benzobicyclobutanes derived from Diels-Alder adduct of 2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TNF-α, IL-8)  
RN 439798-70-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 3-[[[(2,4-dimethoxyphenyl)methyl]amino]carbonyl]-1,2,3,4-tetrahydro-6-methoxy-9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 439798-71-7 CAPLUS  
 CN 1,4-Ethanonaphthalene-2-carboxylic acid, 3-[(dipentylamino)carbonyl]-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

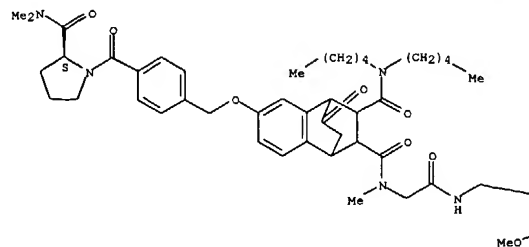
Relative stereochemistry.



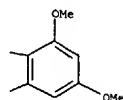
RN 439919-18-3 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxamide, 6-[[4-[[[(2S)-2-[(dimethylamino)carbonyl]-1-pyrrolidinyl]carbonyl]phenyl]methoxy]-1,2,3,4-tetrahydro-N2-methyl-9-oxo-N2-[2-oxo-2-[[[(2,4,6-trimethoxyphenyl)methyl]amino]ethyl]-N3,N3-dipentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



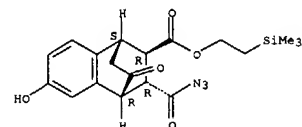
PAGE 1-B



L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
 AB A novel series of TNF- $\alpha$  inhibitors based on a benzobicyclooctane scaffold was reported. The compds. displayed good potency in inhibiting TNF- $\alpha$  induced apoptosis and NF $\kappa$ B activation. Addnl., they were selective for TNF- $\alpha$  as they did not inhibit apoptosis induced by soluble Fas ligand. The compds. described here can act as leads for future medicinal chemical efforts and may also be useful tools for elucidating the TNF- $\alpha$  signaling pathway.  
 ACCESSION NUMBER: 2002:211239 CAPLUS  
 DOCUMENT NUMBER: 137:288467  
 TITLE: Benzobicyclooctanes as novel inhibitors of TNF- $\alpha$  signaling  
 AUTHOR(S): Jackson, Randy W.; Gelinas, Richard; Baughman, Ted A.; Cox, Thomas; Howbert, J. Jeffry; Kucera, Kristin A.; Latham, John A.; Ramsdell, Fred; Singh, Devinder; Darwish, Ihab S.  
 CORPORATE SOURCE: Department of Chemical Genomics, Celltech R&D, Inc., Bothell, WA, 98021, USA  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(7), 1093-1097  
 CODEN: BMCL88; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

IT 439798-79-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (benzobicyclooctanes as novel inhibitors of TNF- $\alpha$  signaling)  
 RN 439798-79-5 CAPLUS  
 CN 1,4-Ethanonaphthalene-2-carboxylic acid, 3-(azidocarbonyl)-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

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COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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SINCE FILE ENTRY	TOTAL SESSION
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SINCE FILE ENTRY	TOTAL SESSION
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STRUCTURE FILE UPDATES: 26 APR 2004 HIGHEST RN 676992-14-6  
DICTIONARY FILE UPDATES: 26 APR 2004 HIGHEST RN 676992-14-6

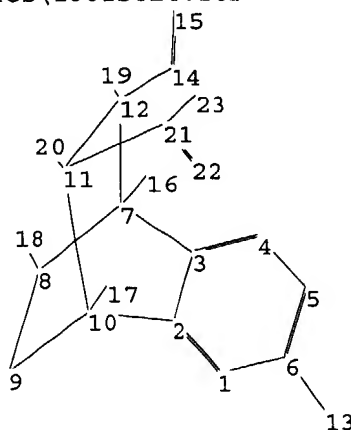
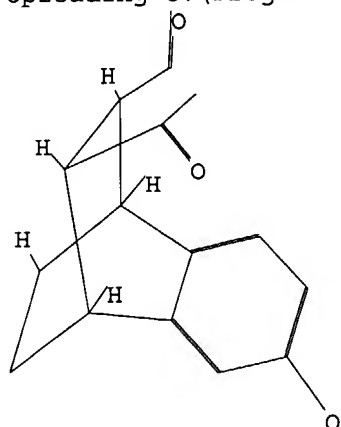
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10015828.str



chain nodes :

13 14 15 16 17 18 19 20 21 22 23

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

6-13 7-16 8-18 10-17 11-20 11-21 12-14 12-19 14-15 21-22 21-23

ring bonds :

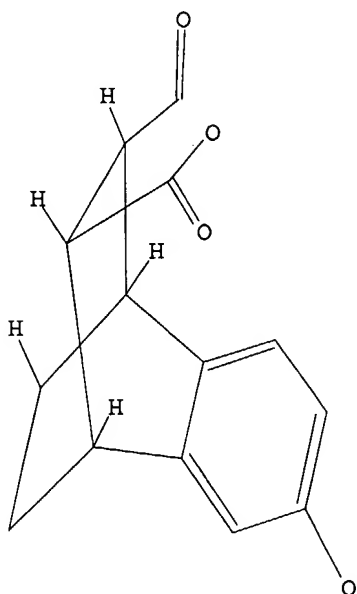
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exact/norm bonds :  
 2-10 3-7 6-13 7-8 7-12 8-9 9-10 10-11 11-12 14-15 21-22  
 exact bonds :  
 7-16 8-18 10-17 11-20 11-21 12-14 12-19 21-23  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS

L10 STRUCTURE UPLOADED

=> d query  
 L10 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l10  
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 SAMPLE SCREEN SEARCH COMPLETED - 415 TO ITERATE

100.0% PROCESSED 415 ITERATIONS  
 SEARCH TIME: 00.00.01

7 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 7078 TO 9522  
 PROJECTED ANSWERS: 7 TO 298



L11 7 SEA SSS SAM L10

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FULL SEARCH INITIATED 17:34:01 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 8193 TO ITERATE

100.0% PROCESSED 8193 ITERATIONS 122 ANSWERS  
SEARCH TIME: 00.00.01

L12 122 SEA SSS FUL L10

=> fil caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	155.42	501.96
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.78

FILE 'CAPLUS' ENTERED AT 17:34:05 ON 27 APR 2004  
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FILE COVERS 1907 - 27 Apr 2004 VOL 140 ISS 18  
FILE LAST UPDATED: 26 Apr 2004 (20040426/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L13 5 L12  
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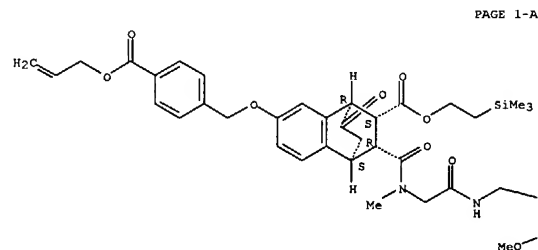
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [R1 = NR8COR9, NR8CO2R9, NR8CON(R9)2, COR9, CO2R9, CON(R9)2; R2 = OR9, N(R9)2; R3 = H, halo, OH, protected-OH, NH2, protected-NH2, alkyl, haloalkyl; R4-5 = R9, OR9, N(R9)2, NNR9, R4, R5 may together form =O, =C(R8)2, NR10 or R4-5 together with the carbon to which they are both attached form spiro carbocyclic or heterocyclic ring; R6 = H, inorg. groups having 1-8 atoms selected from boron, sulfur, phosphorous, silicon, hydrogen, and organic groups having 1-20 carbons, optionally containing 1-4 heteroatoms selected from nitrogen, oxygen and silicon; R7 = halo, OH, protected-OH, NH2, protected-NH2, alkyl, haloalkyl; R8 = H, alkyl, aryl, heteroalkyl; R9 = H, organic groups having 1-30 carbons with the provision that two R9 groups both joined to common atom may be joined together so as to form ring with the common atom; R10 = R9, OR9, N(R9)2, NHCOR9, NHCOR9R9, NHC8NHR9; n is 0-2 with the proviso that when R6 = H, R4-5 together form =O and R1 = CO2R2, then R2 is not OCH3] were prepared for instance, 2,7-dihydroxynaphthalene was reacted with maleic anhydride (1,2-dichlorobenzene/PhMe, 110°C, 3 days) to afford the bicyclobenzocyclobutane adduct (16% yield). This anhydride was reacted with 2-(trimethylsilyl)ethanol affording a 1:1 mixture of regio isomers which was isolated as the dicyclohexylamine (DCA) salt (93% yield). The DCA salt was treated with 2M HCl permitting the isolation of the free regioisomers which were then converted to the isopropylamine salts and crystallized affording the desired regioisomer as a 87/16 mixture. Further crystallization and liberation of the acid ester afforded II as a white solid in 30% overall yield with 98.2% purity by HPLC. Also described is a process of preparing a combinatorial library of I from III [linker = e.g., O-CH2-C6H5-O-CH2CONH; SS = solid support; PG1 = protecting group, e.g., O-allyl; PG2 = protecting group, e.g., OCH2CH2TMS]. The method involves removal of PG1 (PG1 = O-allyl, (Ph3)4Pd/N-methylaniline) in the presence of PG2 (PG2 = OCH2CH2TMS, TBAF) and subsequent amidation with a plurality of amines; removal of PG2 and amidation with a plurality of amines and removal of the linker (TFAaq) to liberate the corresponding bis(amides). A library of 1152 bis(amides) were prepared in this manner. Compds. of the invention were evaluated for inhibition of apoptosis and NFkB. I are useful for inhibiting cellular events involving TNF-α and IL-8, and in the treatment of inflammation events in general.

ACCESSION NUMBER: 2002:504796 CAPLUS  
DOCUMENT NUMBER: 137:78768  
TITLE: Preparation and use of benzobicyclobutanes as inhibitors of TNF-α, IL-8 and for treating inflammation  
INVENTOR(S): Jackson, Randy W.; Darwish, Ihab; Baughman, Ted A.; Howbert, J. Jeffery

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
RN 439798-65-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-3-[[methyl[2-oxo-2-[(2,4,6-trimethoxyphenyl)methyl]amino]ethyl]amino]carbonyl]-10-oxo-7-[[4-[(2-propenyloxy)carbonyl]phenyl]methoxy]-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



PAGE 1-A

RN 439798-68-2 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-[(2,4-dimethoxyphenyl)methyl] 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Page 18

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
PATENT ASSIGNEE(S): Celltech R & D, Inc., USA  
SOURCE: PCT Int. Appl., 200 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

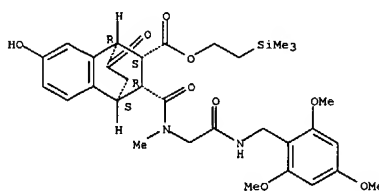
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002051851	A2	20020704	WO 2001-0547993	20011211
WO 2002051851	A3	20030123		

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US 2003069305 A1 20030410 US 2001-15828 20011211  
PRIORITY APPL. INFO.: MARPAT 137:78768  
OTHER SOURCE(S): IT 439798-64-8P 439798-65-9P 439798-66-2P 439798-72-8P 439798-78-4P 439798-92-2P 439799-40-3P 439799-41-4P 439799-45-8P 439799-84-5P 439799-86-7P 439799-90-3P  
RI: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (drug; preparation of benzobicyclobutanes derived from Diels-Alder adduct of 2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TNF-α, IL-8)

RN 439798-64-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-7-hydroxy-3-[[methyl[2-oxo-2-[(2,4,6-trimethoxyphenyl)methyl]amino]ethyl]amino]carbonyl]-10-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

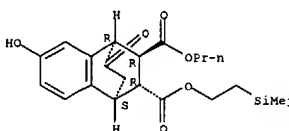
Relative stereochemistry.



L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

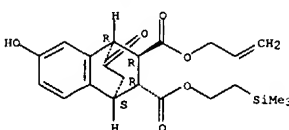
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Relative stereochemistry.



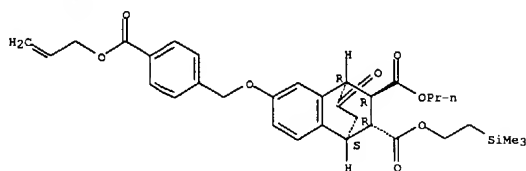
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Relative stereochemistry.



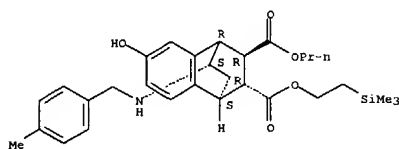
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Relative stereochemistry.



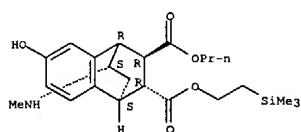
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1,2,3,4-tetrahydro-6-hydroxy-  
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ester, (1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



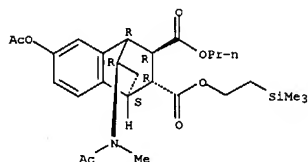
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CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-(methylamino)-, 3-propyl 2-[(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 439799-45-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(acetylmethylamino)-6-  
(acetyloxy)-1,2,3,4-tetrahydro-, 3-propyl 2-[(trimethylsilyl)ethyl]  
ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



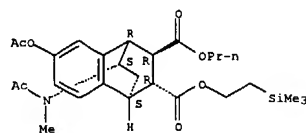
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(drug; preparation of benzobicyclobutanes derived from Diels-Alder  
adduct of  
2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of  
TNF- $\alpha$ , IL-8)

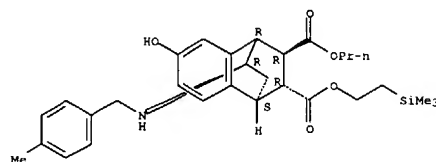
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2-[(trimethylsilyl)ethyl]  
ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



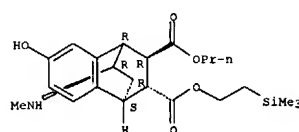
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CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
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9-[[4-methylphenyl)methyl]amino]-, 3-propyl 2-[(trimethylsilyl)ethyl]  
ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



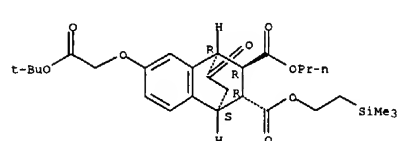
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CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
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Relative stereochemistry.



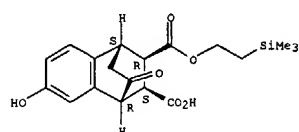
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CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(acetylmethylamino)-6-  
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Relative stereochemistry.



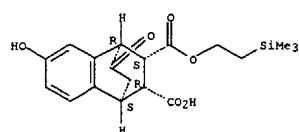
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CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 2-[(2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel- (9CI) (CA  
INDEX NAME)

Relative stereochemistry.



RN 439798-62-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 3-[(2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel- (9CI) (CA  
INDEX NAME)

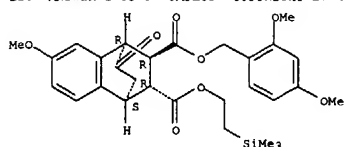
Relative stereochemistry.



RN 439798-69-3 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-methoxy-  
9-oxo-, 3-[(2,4-dimethoxyphenyl)methyl] 2-[(2-(trimethylsilyl)ethyl]  
ester,  
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

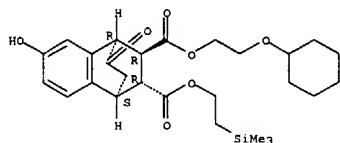
Relative stereochemistry.

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



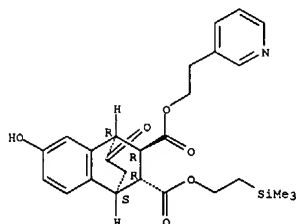
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CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-[2-(cyclohexyloxy)ethyl] 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



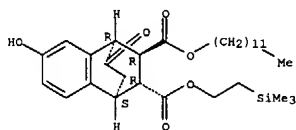
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Relative stereochemistry.



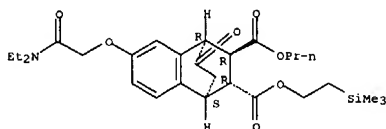
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L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



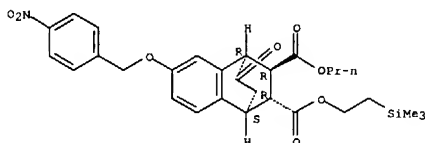
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Relative stereochemistry.



RN 439798-94-4 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-[(4-nitrophenyl)methoxy]-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



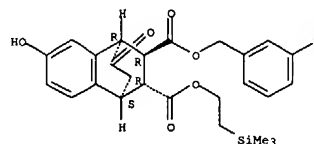
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CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-[(1,1'-biphenyl)-4-ylmethoxy]-1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

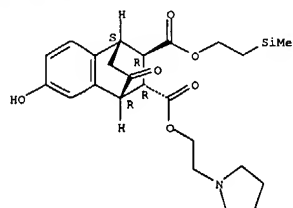
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-[(3-fluorophenyl)methyl] 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 439798-76-2 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-[2-(1-pyrrolidinyl)ethyl] 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

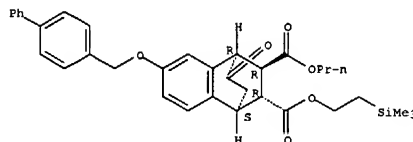
Relative stereochemistry.



RN 439798-77-3 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-dodecyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

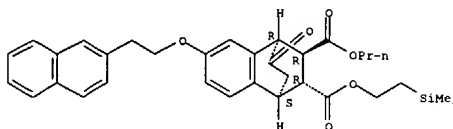
Relative stereochemistry.

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



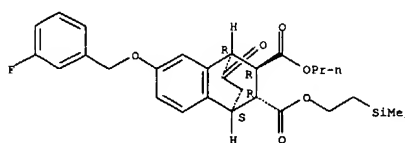
RN 439798-96-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-[2-(2-naphthalenyl)ethoxy]-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



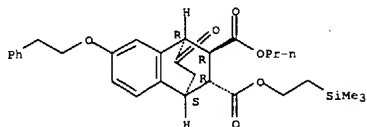
RN 439798-97-7 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-[(3-fluorophenyl)methoxy]-1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



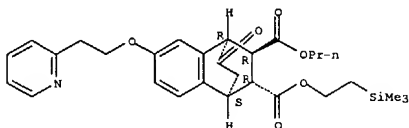
RN 439798-98-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-9-oxo-6-[(2-phenylethoxy)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



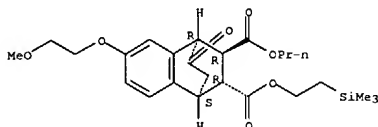
RN 439798-99-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-9-oxo-6-(2-(2-pyridinyl)ethoxy)-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



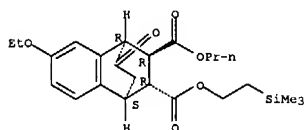
RN 439799-00-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-[(2-methoxyethoxy)-9-oxo-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



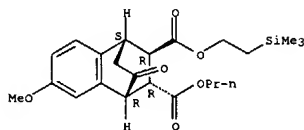
RN 439799-01-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-(cyclopentyloxy)-1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



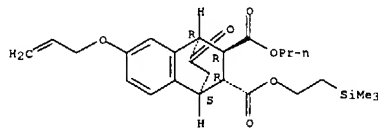
RN 439799-05-0 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-methoxy-9-oxo-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



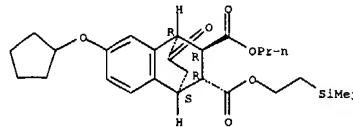
RN 439799-06-1 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-9-oxo-6-(2-propenyl)ethoxy-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



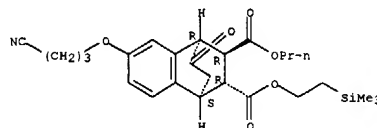
RN 439799-07-2 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-9-oxo-6-(3-pyridinylmethoxy)-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



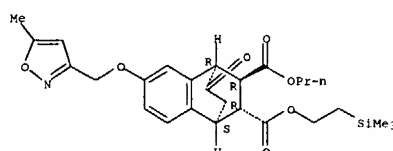
RN 439799-02-7 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-(3-cyanopropoxy)-1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



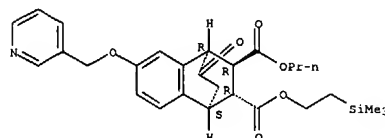
RN 439799-03-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-[(5-methyl-3-isoxazolyl)methoxy]-9-oxo-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



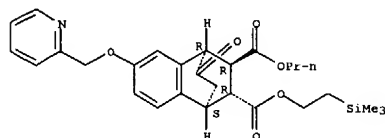
RN 439799-04-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-ethoxy-1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



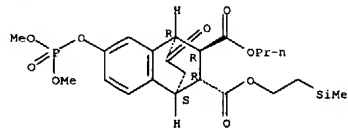
RN 439799-08-3 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-9-oxo-6-(2-pyridinylmethoxy)-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 439799-09-4 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-[(dimethoxyphosphinyl)oxy]-1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

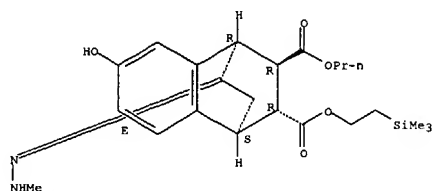
Relative stereochemistry.



RN 439799-11-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-(methylhydrazono)-, 3-propyl 2-[(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S,9E)-rel- (9CI) (CA INDEX NAME)

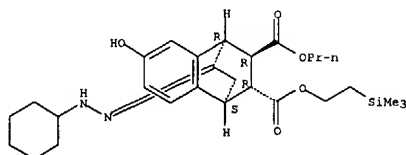
Relative stereochemistry.

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
Double bond geometry as shown.



RN 439799-12-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(cyclohexylhydrazono)-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.

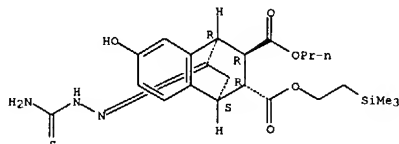


RN 439799-13-0 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[(2-bromophenyl)hydrazono]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.

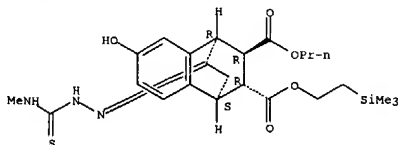
L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Relative stereochemistry.  
Double bond geometry unknown.



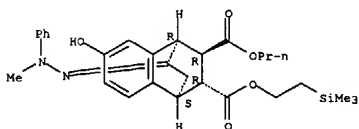
RN 439799-17-4 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-[(methylamino)thioxomethyl]hydrazono]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-18-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-(methylphenylhydrazono)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

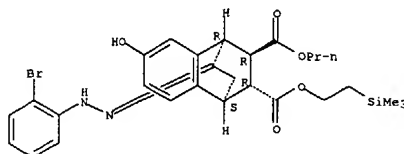
Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-19-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[(4-methoxyphenyl)sulfonyl]hydrazono]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

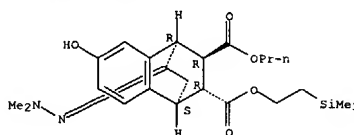
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L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



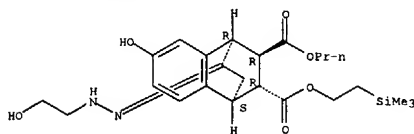
RN 439799-14-1 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(dimethylhydrazono)-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-15-2 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-5-[(2-hydroxyethyl)hydrazono]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

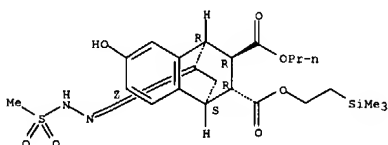
Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-16-3 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[(aminothioxomethyl)hydrazono]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

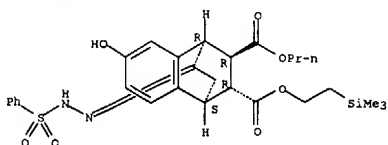
L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
9-[(methylsulfonyl)hydrazono]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9Z)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry as shown.



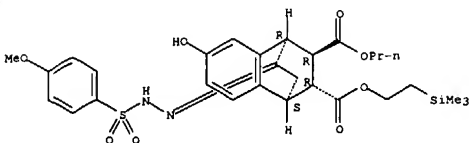
RN 439799-20-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-[(phenylsulfonyl)hydrazono]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-21-0 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-[(4-methoxyphenyl)sulfonyl]hydrazono]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.

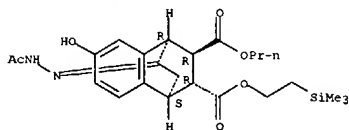


L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 439799-22-1 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(acetylhydrazono)-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

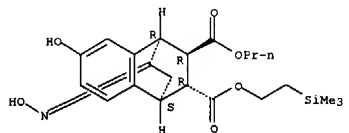
Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-23-2 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-(hydroxyimino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-24-3 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-(methoxyimino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9E)-rel- (9CI) (CA INDEX NAME)

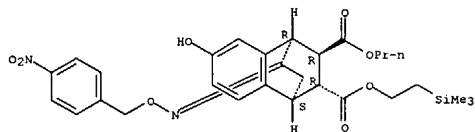
Relative stereochemistry.  
Double bond geometry as shown.



L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

9-[[[4-nitrophenyl)methoxy]imino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

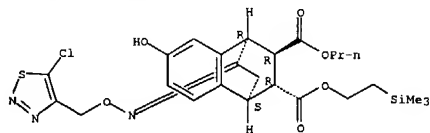
Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-28-7 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[[[5-chloro-1,2,3-thiadiazol-4-yl)methoxy]imino]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

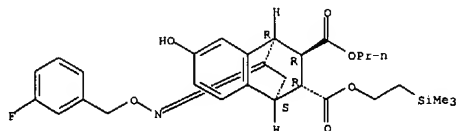
Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-29-8 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[[[3-fluorophenyl)methoxy]imino]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.

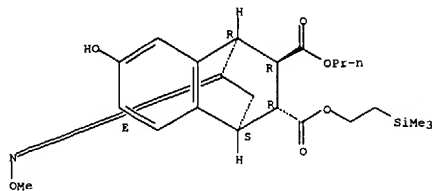


RN 439799-30-1 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-

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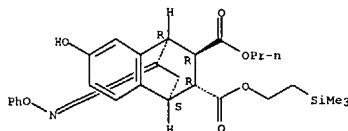
L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 439799-25-4 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-(phenoxyimino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

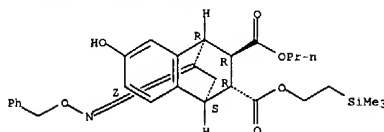
Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-26-5 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-[1-(phenylmethoxy)imino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9Z)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry as shown.



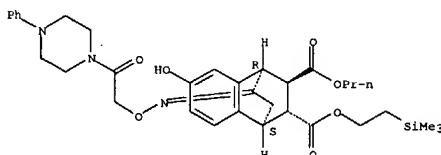
RN 439799-27-6 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

9-[[2-oxo-2-(4-phenyl-1-piperazinyl)ethoxy]imino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9E)-rel- (9CI) (CA INDEX NAME)

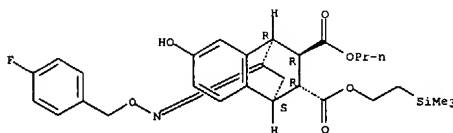
Relative stereochemistry.  
Double bond geometry as shown.



RN 439799-31-2 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[[[4-fluorophenyl)methoxy]imino]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

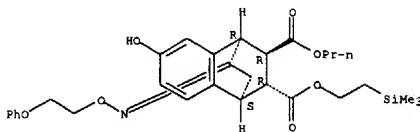
Relative stereochemistry.  
Double bond geometry unknown.



RN 439799-32-3 CAPLUS

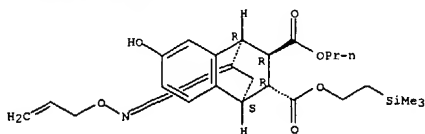
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-[[2-(phenoxyethoxy)imino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.



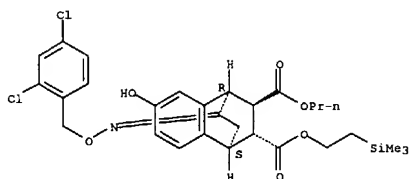
RN 439799-33-4 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-[(2-propenyloxy)imino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.



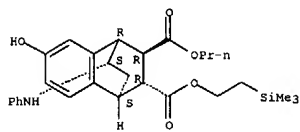
RN 439799-34-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[(2,4-dichlorophenyl)methoxyimino]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9E)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry as shown.



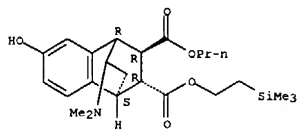
RN 439799-35-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[(aminocarbonyl)hydrazone]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.



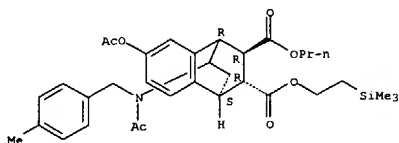
RN 439799-43-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(dimethylamino)-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



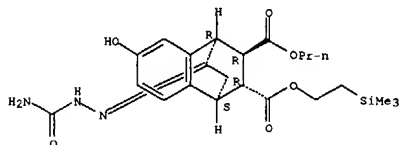
RN 439799-44-7 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[acetyl[(4-methylphenyl)methyl]amino]-6-(acetyloxy)-1,2,3,4-tetrahydro-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



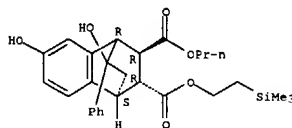
RN 439799-46-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(acetylmethylamino)-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



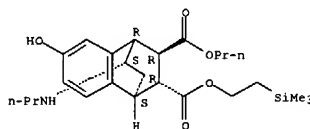
RN 439799-38-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-9-phenyl-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



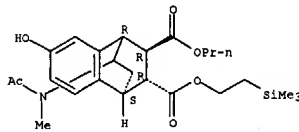
RN 439799-39-0 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-(propylamino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



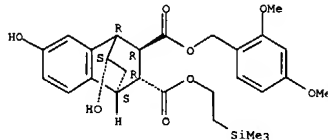
RN 439799-42-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-(phenylamino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

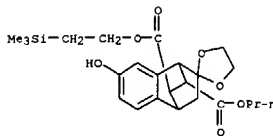


RN 439799-48-1 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-, 3-[(2,4-dimethoxyphenyl)methyl] 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



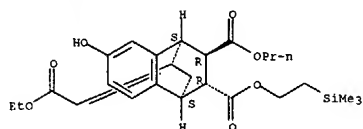
RN 439799-49-2 CAPLUS  
CN Spiro[1,3-dioxolane-2,2'-(1'H)-[1,4]ethanonaphthalene]-9',10'-dicarboxylic acid, 3',4'-dihydro-7'-hydroxy-, 10'-propyl 9'-[2-(trimethylsilyl)ethyl] ester, (1'R,4'S,9'R,10'R)-rel- (9CI) (CA INDEX NAME)



RN 439799-50-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(2-ethoxy-2-oxoethylidene)-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

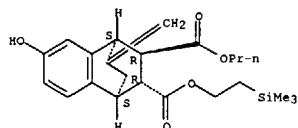
Relative stereochemistry.  
Double bond geometry unknown.





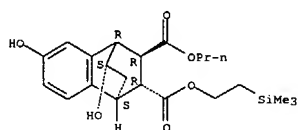
RN 439799-51-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-methylene-, 3-propyl 2-[(2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



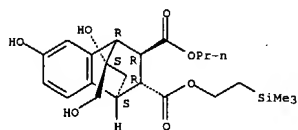
RN 439799-52-7 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-  
dihydroxy-, 3-propyl 2-[(2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



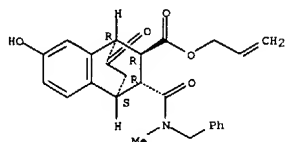
RN 439799-53-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
9-amino-1,2,3,4-tetrahydro-6-  
hydroxy-, 3-propyl 2-[(2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel-  
(9CI) (CA INDEX NAME)

Relative stereochemistry.



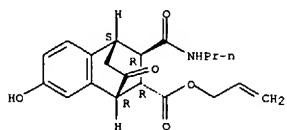
RN 439799-59-4 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-7-hydroxy-3-  
[[methyl(phenylmethyl)amino]carbonyl]-10-oxo-, 2-propenyl ester,  
(1R,2R,3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



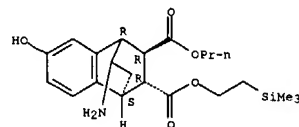
RN 439799-60-7 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-7-hydroxy-10-  
oxo-3-[(propylamino)carbonyl]-, 2-propenyl ester, (1R,2R,3R,4S)-rel-  
(9CI) (CA INDEX NAME)

Relative stereochemistry.



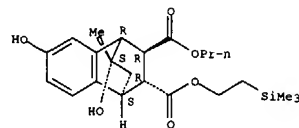
RN 439799-64-1 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 2-[[2-[(4-methylphenyl)sulfonyl]ethyl] 3-propyl ester,  
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



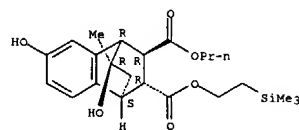
RN 439799-54-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-  
dihydroxy-9-methyl-, 3-propyl 2-[(2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



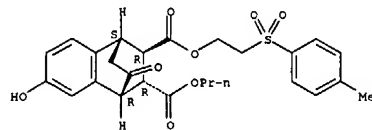
RN 439799-56-1 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-  
dihydroxy-9-methyl-, 3-propyl 2-[(2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



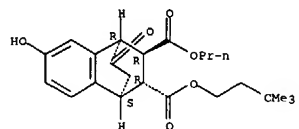
RN 439799-58-3 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-  
dihydroxy-9-(hydroxymethyl)-, 3-propyl 2-[(2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



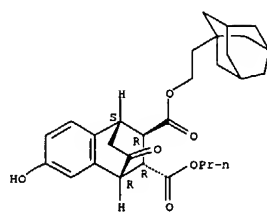
RN 439799-66-3 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 2-[(3,3-dimethylbutyl) 3-propyl ester, (1R,2S,3S,4S)-rel- (9CI)  
(CA INDEX NAME)

Relative stereochemistry.



RN 439799-68-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 3-propyl 2-[(2-tricyclo[3.3.1.1.3,7]dec-1-ylethyl] ester,  
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

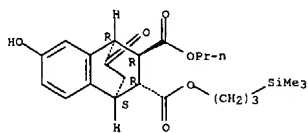
Relative stereochemistry.



RN 439799-69-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-

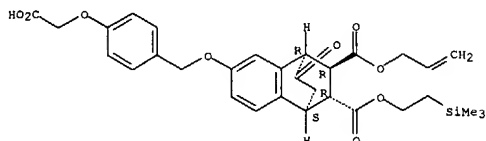
L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
 9-oxo-, 3-propyl 2-[3-(trimethylsilyl)propyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



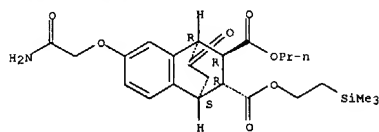
RN 439799-71-0 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-[[4-(carboxymethoxy)phenyl]methoxy]-1,2,3,4-tetrahydro-9-oxo-, 3-(2-propenyl) 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



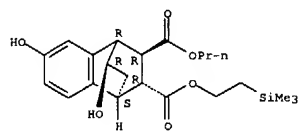
RN 439799-75-4 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-(2-amino-2-oxoethoxy)-1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



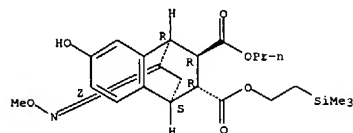
RN 439799-77-6 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-(3-hydroxypropoxy)-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



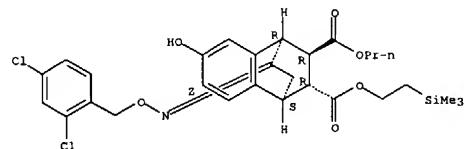
RN 439800-16-5 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[(2,4-dichlorophenyl)methoxymethyl]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



RN 439800-17-6 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[(2,4-dimethoxyphenyl)methoxymethyl]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

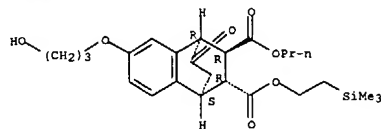
Relative stereochemistry.  
 Double bond geometry as shown.



RN 439800-18-7 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-, 3-[(2,4-dimethoxyphenyl)methyl] 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

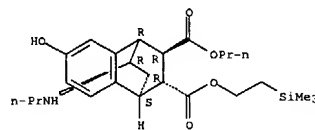
Relative stereochemistry.

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
 Relative stereochemistry.



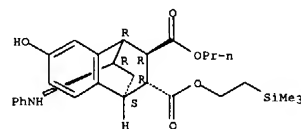
RN 439799-82-3 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-, 9-(propylamino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 439799-88-9 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-, 9-(phenylamino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

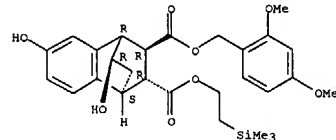
Relative stereochemistry.



RN 439799-91-4 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

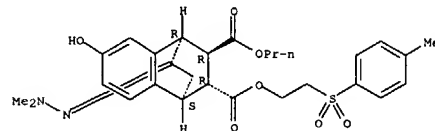
Relative stereochemistry.

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



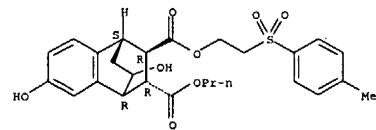
RN 439800-20-1 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(dimethylhydrazono)-1,2,3,4-tetrahydro-6-hydroxy-, 2-[2-[(4-methylphenyl)sulfonyl]ethyl] 3-propyl ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry unknown.



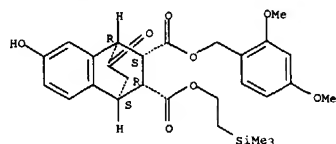
RN 439800-21-2 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-, 2-[2-[(4-methylphenyl)sulfonyl]ethyl] 3-propyl ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



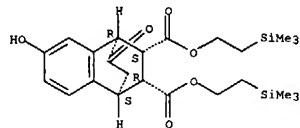
RN 439800-22-3 CAPLUS  
 CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-, 9-oxo-, 3-[(2,4-dimethoxyphenyl)methyl] 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



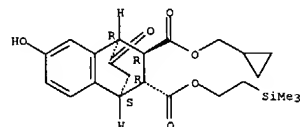
RN 439800-23-4 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, bis[2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 439800-24-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 3-(cyclopropylmethyl) 2-[2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

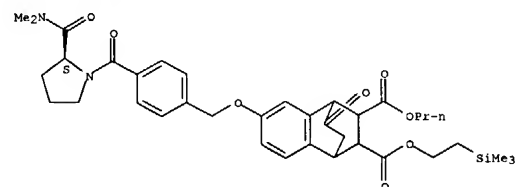


RN 439800-26-7 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-[(methoxycarbonyl)hydrazono]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.

L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
tetrahydro-9-oxo-, 3-propyl 2-(trimethylsilyl)ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 439799-94-7P 439799-96-9P 439800-03-0P  
439800-13-2P 439800-19-8P 439800-29-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Intermediate; preparation of benzobicyclobutanes derived from Diels-Alder adduct of 2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TNF- $\alpha$ , IL-8)

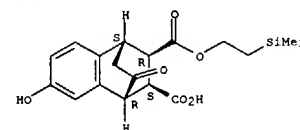
RN 439799-94-7 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel-, compd.

with N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

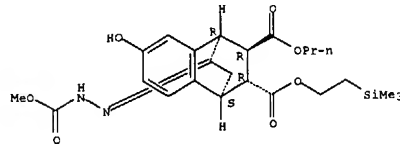
CRN 439798-61-5  
CMF C19 H24 O6 Si

Relative stereochemistry.



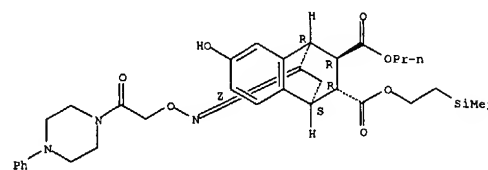
CM 2

CRN 101-83-7  
CMF C12 H23 N



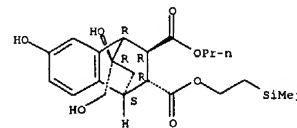
RN 439800-27-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-[[[2-oxo-2-(4-phenyl-1-piperazinyl)ethoxy]imino]-, 3-propyl  
2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9Z)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry as shown.

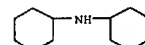


RN 439800-28-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-9-(hydroxymethyl)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 439919-19-4 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-[[4-[(2S)-2-[(dimethylamino)carbonyl]-1-pyrrolidinyl]carbonyl]phenyl]methoxy]-1,2,3,4-

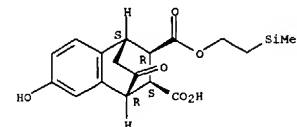


RN 439799-96-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel-, compd.  
with 2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

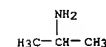
CRN 439798-61-5  
CMF C19 H24 O6 Si

Relative stereochemistry.



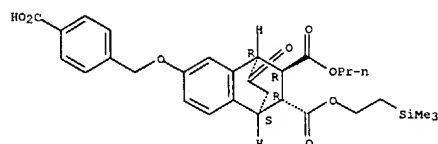
CM 2

CRN 75-31-0  
CMF C3 H9 N



RN 439800-03-0 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
6-[[4-carboxyphenyl]methoxy]-  
1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

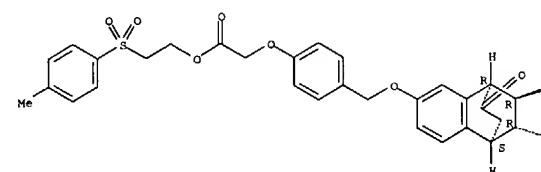
Relative stereochemistry.



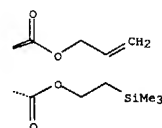
RN 439800-13-2 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-[[4-[[2-[[2-[[4-methylphenyl)sulfonyl]ethoxy]-2-oxoethoxy]phenyl]methoxy]-9-oxo-, 3-(2-propenyl) 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI)  
(CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



RN 439800-19-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-[[[4-methylphenyl)methyl]amino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl]

AB A novel series of TNF- $\alpha$  inhibitors based on a benzobicyclooctane scaffold was reported. The comps. displayed good potency in inhibiting TNF- $\alpha$  induced apoptosis and NF $\kappa$ B activation. Addnl., they were selective for TNF- $\alpha$  as they did not inhibit apoptosis induced by soluble Fas ligand. The comps. described here can act as leads for future medicinal chemical efforts and may also be useful tools for elucidating the TNF- $\alpha$  signaling pathway.

ACCESSION NUMBER: 2002:211239 CAPLUS  
DOCUMENT NUMBER: 137:288467  
TITLE: Benzobicyclooctanes as novel inhibitors of TNF- $\alpha$  signaling  
AUTHOR(S): Jackson, Randy W.; Gelinas, Richard; Baughman, Ted A.;  
Cox, Thomas; Howbert, J. Jeffery; Kucera, Kristin A.; Latham, John A.; Ramsdell, Fred; Singh, Devinder;

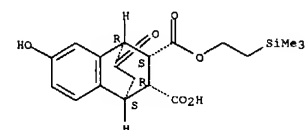
CORPORATE SOURCE: Darwish, Zhab S.  
Department of Chemical Genomics, Celltech R&D, Inc., Bothell, WA, 98021, USA  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(7), 1093-1097  
CODEN: BMCLES; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

IT 439798-62-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(att obbenzobicyclooctanes as novel inhibitors of TNF- $\alpha$  signaling)

RN 439798-62-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

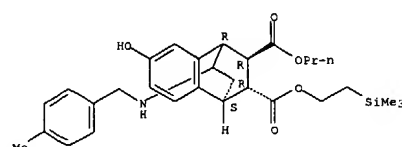
Relative stereochemistry.



IT 439798-72-8P 439798-75-1P 439798-78-4P 439799-66-3P 439799-69-6P 468086-81-9P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(benzobicyclooctanes as novel inhibitors of TNF- $\alpha$  signaling)

RN 439798-72-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

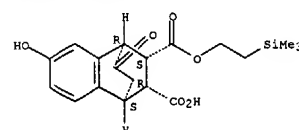


RN 439800-29-0 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

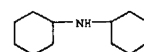
CRN 439798-62-6  
CMF C19 H24 O6 Si

Relative stereochemistry.

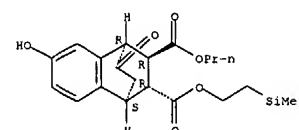


CM 2

CRN 101-83-7  
CMF C12 H23 N

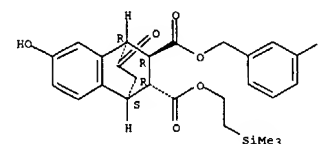


Relative stereochemistry.



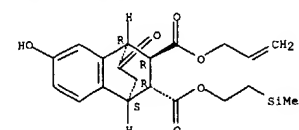
RN 439798-75-1 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-[[3-(fluorophenyl)methyl] 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



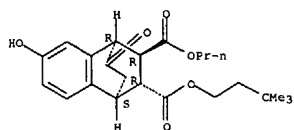
RN 439798-78-4 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-[2-(propenyl) 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



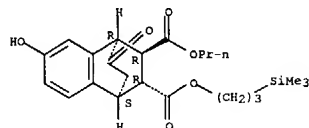
RN 439799-66-3 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-[3,3-dimethylbutyl] 3-propyl ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

L13 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)  
Relative stereochemistry.



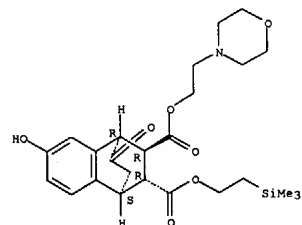
RN 439799-69-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 3-propyl 2-[3-(trimethylsilyl)propyl] ester, (1R,2S,3S,4S)-rel-  
(9CI) (CA INDEX NAME)

Relative stereochemistry.



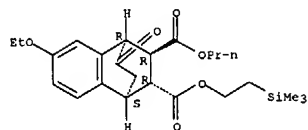
RN 468086-81-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 3-[2-(4-morpholinyl)ethyl] 2-[2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



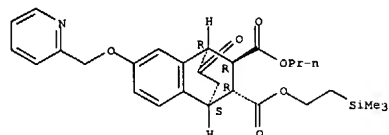
IT 364778-17-6P 439798-99-9P 439799-04-9P

L13 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



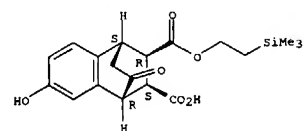
RN 439799-08-3 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-9-oxo-6-(2-  
pyridinylmethoxy)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 439798-61-5P 468086-79-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(benzobicyclooctanes as novel inhibitors of TNF-α signaling)  
RN 439798-61-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel- (9CI) (CA  
INDEX NAME)

Relative stereochemistry.



RN 468086-79-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-hydroxy-  
9-oxo-, 3-propyl ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

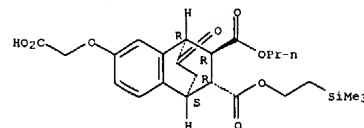
Page 29

L13 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

439799-08-3P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

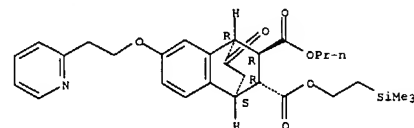
(benzobicyclooctanes as novel inhibitors of TNF-α signaling)  
RN 364778-17-6 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-(carboxymethoxy)-1,2,3,4-  
tetrahydro-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 439798-99-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-9-oxo-6-[2-  
(2-pyridinyl)ethoxy]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,  
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

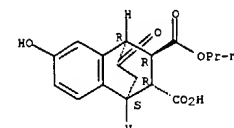


RN 439799-04-9 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
6-ethoxy-1,2,3,4-tetrahydro-9-  
oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel-  
(9CI) (CA INDEX NAME)

Relative stereochemistry.

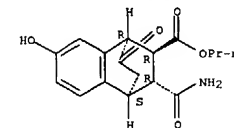
L13 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Relative stereochemistry.



IT 468086-80-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(benzobicyclooctanes as novel inhibitors of TNF-α signaling)  
RN 468086-80-8 CAPLUS  
CN 1,4-Ethanonaphthalene-2-carboxylic acid, 3-(aminocarbonyl)-1,2,3,4-  
tetrahydro-7-hydroxy-10-oxo-, propyl ester, (1R,2R,3R,4S)-rel- (9CI) (CA  
INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L13 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

AB A method for the preferred cleavage of t-Bu esters with silica gel in refluxing toluene is reported. Good yields of the corresponding carboxylic acids are obtained, and the reaction is selective for t-Bu esters over t-Bu ethers and (trimethylsilyl)ethyl esters.

ACCESSION NUMBER: 2001:50189 CAPLUS

DOCUMENT NUMBER: 135:288318

TITLE: A mild and selective method for the cleavage of

AUTHOR(S): tert-butyl esters

CORPORATE SOURCE: Jackson, R. W.

SOURCE: Department of Chemical Genomics, Celltech R&D, Inc.,

Bothell, WA, 98021, USA

Tetrahedron Letters (2001), 42(31), 5163-5165

CODEN: TETLEA; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:288318

IT 364778-16-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of carboxylic acids via a mild and selective method for

the cleavage of tert-Bu esters)

RN 364778-16-5 CAPLUS

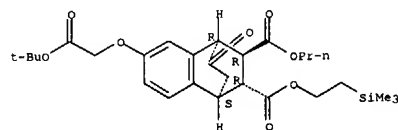
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-[2-(1,1-dimethylethoxy)-2-

oxoethoxy]-1,2,3,4-tetrahydro-9-oxo-, 3-propyl

2-[2-(trimethylsilyl)ethyl]

ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 364778-17-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of carboxylic acids via a mild and selective method for

the cleavage of tert-Bu esters)

RN 364778-17-6 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-(carboxymethoxy)-1,2,3,4-

tetrahydro-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,

(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L13 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

AB In methoxybenzobicyclo[2.2.2]octen-2-one derivs. a change in the position of the MeO group causes a change in the direction of the transition dipole

moment without much alteration in the  $\sigma$ -electron distribution. The effects of the change of the direction of the local chromophore on the optical activity were studied and analyzed by the application of dynamic and static coupling mechanisms. The optical activity is mainly produced by vector- $\mu$ -vector-m coupling and depends on the direction of the local transition moments.

ACCESSION NUMBER: 1978:169387 CAPLUS

DOCUMENT NUMBER: 88:169387

TITLE: Optical activity in  $\beta$ -unsaturated ketones.

Part 1. Effect of the direction of the electric

transition dipole moment in the aromatic group in

benzobicyclo[2.2.2]octen-2-one derivatives

Hagishita, Sanji; Kuriyama, Kaoru

Shionogi Res. Lab., Shionogi and Co. Ltd., Osaka,

JAPAN

SOURCE: Journal of the Chemical Society, Perkin Transactions

2: Physical Organic Chemistry (1972-1999) (1977),

(14), 1937-41

CODEN: JCPKBN; ISSN: 0300-9580

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 66289-18-7

RL: PRP (Properties)

(optical activity of, elec. transition dipole moment in relation to)

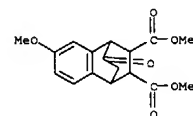
RN 66289-18-7 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,

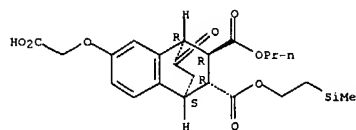
1,2,3,4-tetrahydro-6-methoxy-

9-oxo-, dimethyl ester, (1 $\alpha$ ,2 $\beta$ ,3 $\alpha$ ,4 $\alpha$ )- (9CI) (CA

INDEX NAME)



L13 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS

FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

L13 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

AB The Diels-Alder reaction of 1,7-, 2,7-, 2,6-, and 1,6-dihydroxynaphthalene

and 6-bromo-2-naphthol with maleic anhydride was investigated. All of these 2-naphthol derivs. gave exo and endo adducts except for the bromonaphthol, from which only an endo adduct was obtained. The assignment of exo or endo configuration was based on lactone formation on NaBH4 reduction (possible only from the exo isomer), comparison of NMR spectra, and in some cases dipole moment measurements. The exo-endo ratios of the formed adducts vary over a wide range. Title resolution

was accomplished via the cinchonidine salts. The absolute configuration of

the resolved compds. was determined by applying the octant rule.

ACCESSION NUMBER: 1970:414534 CAPLUS

DOCUMENT NUMBER: 73:14534

TITLE: Diels-Alder reaction. IX. Reaction of 1,7-, 2,7-,

2,6-, and 1,6-dihydroxynaphthalene and

6-bromo-2-naphthol with maleic anhydride and the

resolution of some derivatives of the adducts

Takeda, Kenichi; Hagishita, Sanji; Sugiyama, Michi;

Kitahonoki, Keizo; Ban, Isao; Miyazaki, Sadao;

Kuriyama, Kaoru

Shionogi Res. Lab., Shionogi and Co. Ltd., Osaka,

JAPAN

SOURCE: Tetrahedron (1970), 26(6), 1435-51

CODEN: TETRAH; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 29038-00-4P 29073-46-9P 29073-55-0P

29073-64-1P 29073-71-0P 29196-80-3P

29206-51-7P 31770-13-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

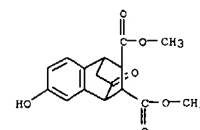
(preparation of)

RN 29038-00-4 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1 $\alpha$ ,2 $\beta$ ,3 $\alpha$ ,4 $\alpha$

pha.-tetrahydro-6-hydroxy-9-oxo-, dimethyl ester, ( $\pm$ )- (8CI) (CA INDEX

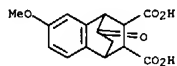
NAME)



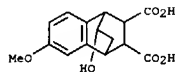
RN 29073-46-9 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1 $\alpha$ ,2 $\beta$ ,3 $\alpha$ ,4 $\alpha$

pha.-tetrahydro-6-methoxy-9-oxo-, ( $\pm$ )- (8CI) (CA INDEX NAME)



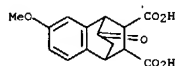
RN 29073-55-0 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1 $\alpha$ ,2 $\beta$ ,3 $\alpha$ ,4.α  
lpha.-tetrahydro-10-hydroxy-6-methoxy-, (±)- (8CI) (CA INDEX NAME)



RN 29073-64-1 CAPLUS  
CN Cinchonidine, (1S,2S,3S,4R)-(+)-1,2,3,4-tetrahydro-6-methoxy-9-oxo-1,4-ethanonaphthalene-2,3-dicarboxylate (1:1) (8CI) (CA INDEX NAME)

CM 1

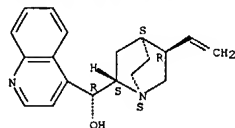
CRN 47131-85-1  
CMF C15 H14 O6



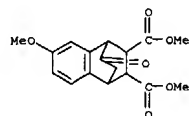
CM 2

CRN 485-71-2  
CMF C19 H22 N2 O

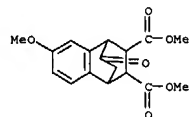
Absolute stereochemistry.



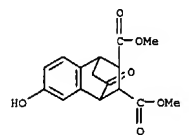
RN 29073-71-0 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1 $\alpha$ ,2 $\beta$ ,3 $\beta$ ,4.α  
lpha.-tetrahydro-6-methoxy-9-oxo-, dimethyl ester, (±)- (8CI) (CA INDEX NAME)



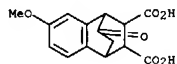
RN 29196-80-3 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1 $\alpha$ ,2 $\alpha$ ,3 $\alpha$ ,4.α  
lpha.-tetrahydro-6-methoxy-9-oxo-, dimethyl ester, (±)- (8CI) (CA INDEX NAME)



RN 29206-51-7 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1 $\alpha$ ,2 $\alpha$ ,3 $\alpha$ ,4.α  
lpha.-tetrahydro-6-hydroxy-9-oxo-, dimethyl ester, (±)- (8CI) (CA INDEX NAME)



RN 31770-13-5 CAPLUS  
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,  
1,2,3,4-tetrahydro-6-methoxy-  
9-oxo-, disodium salt, (1S,2S,3S,4R)-(+)- (8CI) (CA INDEX NAME)



●2 Na

=> fil reg  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
27.72	529.68

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-3.47	-6.25

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 17:39:23 ON 27 APR 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 26 APR 2004 HIGHEST RN 676992-14-6  
DICTIONARY FILE UPDATES: 26 APR 2004 HIGHEST RN 676992-14-6

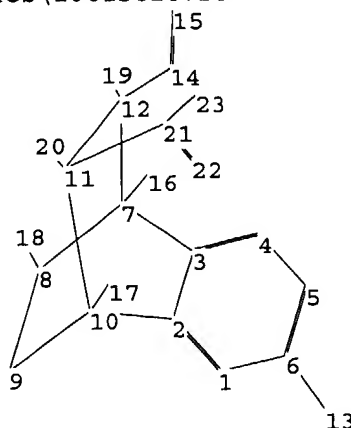
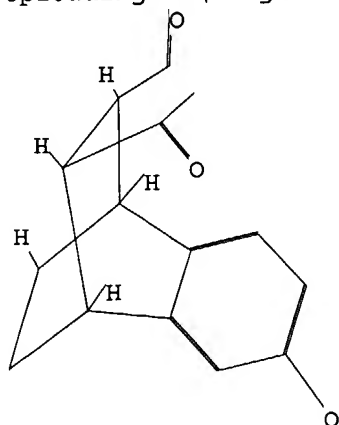
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10015828.str



chain nodes :

13 14 15 16 17 18 19 20 21 22 23

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

6-13 7-16 8-18 10-17 11-20 11-21 12-14 12-19 14-15 21-22 21-23

ring bonds :

1-2 1-6 2-3 2-10 3-4 3-7 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

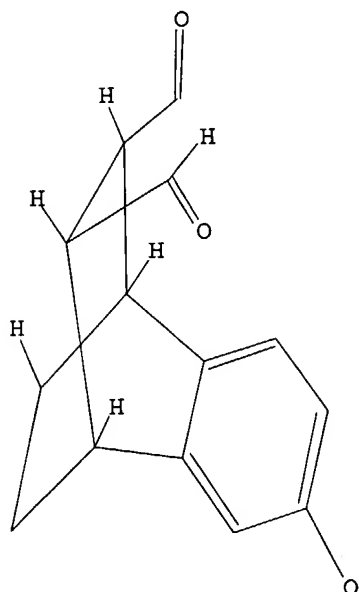


exact/norm bonds :  
 2-10 3-7 6-13 7-8 7-12 8-9 9-10 10-11 11-12 14-15 21-22  
 exact bonds :  
 7-16 8-18 10-17 11-20 11-21 12-14 12-19 21-23  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS

L14 STRUCTURE UPLOADED

=> d query  
 L14 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l14  
 SAMPLE SEARCH INITIATED 17:40:45 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 487 TO ITERATE

100.0% PROCESSED 487 ITERATIONS  
 SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 8417 TO 11063  
 PROJECTED ANSWERS: 0 TO 0

L15 0 SEA SSS SAM L14

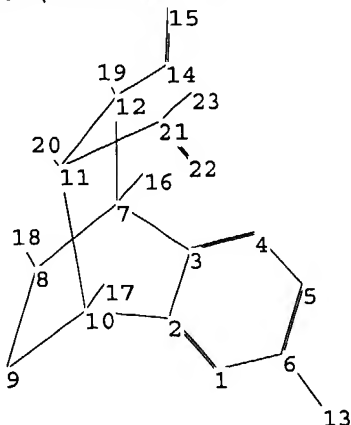
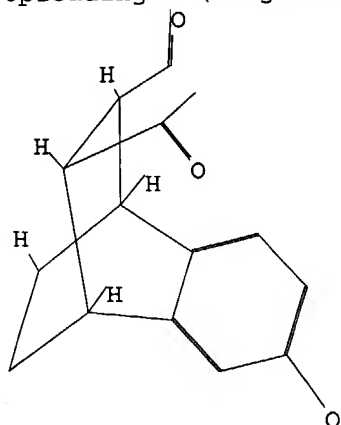
=> s l14 full  
FULL SEARCH INITIATED 17:40:48 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 9873 TO ITERATE

100.0% PROCESSED 9873 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

L16 0 SEA SSS FUL L14

=>  
Uploading C:\Program Files\Stnexp\Queries\10015828.str

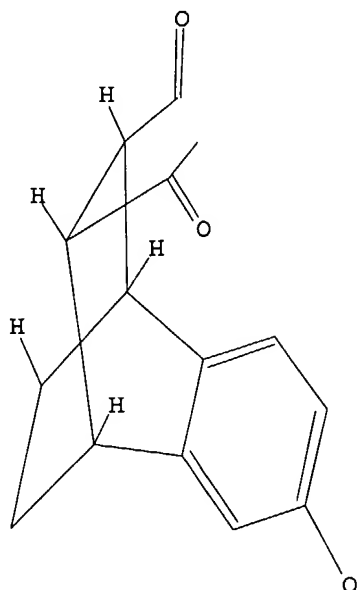


chain nodes :  
13 14 15 16 17 18 19 20 21 22 23  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 12  
chain bonds :  
6-13 7-16 8-18 10-17 11-20 11-21 12-14 12-19 14-15 21-22 21-23  
ring bonds :  
1-2 1-6 2-3 2-10 3-4 3-7 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12  
exact/norm bonds :  
2-10 3-7 6-13 7-8 7-12 8-9 9-10 10-11 11-12 14-15 21-22  
exact bonds :  
7-16 8-18 10-17 11-20 11-21 12-14 12-19 21-23  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS

L17 STRUCTURE UPLOADED

=> d query  
L17 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l17

SAMPLE SEARCH INITIATED 17:44:36 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 120 TO ITERATE

100.0% PROCESSED 120 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 1743 TO 3057  
PROJECTED ANSWERS: 0 TO 0

L18 0 SEA SSS SAM L17

=> s l17 full

FULL SEARCH INITIATED 17:44:40 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 2151 TO ITERATE

100.0% PROCESSED 2151 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

L19 0 SEA SSS FUL L17

=> logoff y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
314.20	843.88

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-6.25

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STN INTERNATIONAL LOGOFF AT 17:45:36 ON 27 APR 2004